

Solution of quantum double exchange on the complete graph from $\text{spl}(2,1)$ dynamical supersymmetry

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The exact and analytical low energy spectrum of the ferromagnetic Kondo lattice model on a complete graph extended with on-site repulsion U is obtained in terms of a dynamical $\text{spl}(2,1)$ supersymmetry in the limit of infinitely strong Hund's coupling (double exchange). Furthermore, we show that for the particular value of $U = J_H/2$ the supersymmetry is not constrained to infinite J_H/t only and we calculate the energy including the t^2/J_H corrections analytically and we give numerical evidence which suggest that the Kondo Hamiltonian is itself supersymmetric for any J_H/t . On a N site graph, the ferromagnetic ground state is realized for 1 and $N+1$ electrons only. In the leading order in the value of the core spin, the quantum and semiclassical spectra are identical.

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The recent experimental activity on manganites, $\text{La}_{1-x}\text{A}_x\text{MnO}_3$ (where $\text{A}=\text{Ca}, \text{Sr}$ or Ba), a family intensively studied due to its colossal magnetoresistance [1], has stimulated the interest of theorists for this compound. While the orbital degrees of freedom certainly cannot be neglected for the real material [2], it is believed that some aspects of the physics of the transition metal oxides can be revealed by considering the Kondo-lattice Hamiltonian $\mathcal{H}_{\text{KL}} = \mathcal{T} + \mathcal{H}_{\text{int}}$, where the kinetic part

$$\mathcal{T} = - \sum_{i,j,\alpha} t_{ij} c_{i\alpha}^\dagger c_{j\alpha}, \quad t_{ij} > 0, \quad (1)$$

describes the hopping of electron on a lattice ($\alpha = \uparrow, \downarrow$ is the spin index), and the interaction part reads

$$\mathcal{H}_{\text{int}} = - \frac{J_H}{2} \sum_{j,\alpha,\beta} c_{j\alpha}^\dagger \mathbf{S}_{cj} \boldsymbol{\sigma}_{\alpha\beta} c_{j\beta} + U \sum_j n_{j\uparrow} n_{j\downarrow}. \quad (2)$$

Here J_H stands for the intratomic ferromagnetic exchange (Hund's coupling) between the conduction electrons and localized core electrons [3], $\boldsymbol{\sigma}_{\alpha\beta}$ denotes the vector of Pauli matrices, and \mathbf{S}_{cj} is the spin operator of the localized core electrons with spin S_c . We also include the on-site Coulomb repulsion $U > 0$ between the electrons, with U of the order of J_H . While here we are interested in $J_H > 0$, the Kondo-lattice Hamiltonian has been extensively studied for $J_H < 0$, as describing heavy fermion systems [4].

Because the Hund coupling is typically larger than the hopping (in manganites $J_H \approx 1 - 2\text{eV}$ and $t \approx 0.1 - 0.5\text{eV}$), the energetically unfavorable low spin states are usually neglected and we get the quantum double exchange, with a rather complicated Hamiltonian [5,6]. The next usually used approximation neglects the quantum spin fluctuation of the S_c core spin replacing it by classical variables (spherical angles θ and ϕ). These two approximations lead to the double-exchange model [6,7] with Hamiltonian $H_{\text{de}} = - \sum_{ij} \tilde{t}_{ij} f_i^\dagger f_j$, which describes noninteracting spinless fermions (charges) moving in a disordered background of classical spins $\tilde{t}_{ij} =$

$$t_{ij} [\cos(\theta_i/2) \cos(\theta_j/2) + \sin(\theta_i/2) \sin(\theta_j/2) e^{i(\phi_i - \phi_j)}].$$

The charges can freely propagate provided the core spins are aligned and therefore ferromagnetism is favored. The main effect of finite J_H is to introduce antiferromagnetic exchange between the core spins, which will hinder the free propagation of the holes, resulting in a competition between ferromagnetic and antiferromagnetic ordering. To check the scenario presented above, different numerical methods, like exact diagonalization, quantum Monte Carlo, density matrix renormalisation group and dynamical mean field are applied [8–11].

Here we will consider the model where the hopping is infinitely long ranged, i.e. complete graph with $t_{ij} = t(1 - \delta_{ij})$. The numerical diagonalizations show that the spectrum separate into well defined bands for large enough J_H . A typical example of the lowest band is shown in Fig. 1 in the case of a small 4-site cluster where states at the right upper corner belong to the next band. It appears that with long ranged hopping, the lowest band is surprisingly simple in the limit $J_H/t \rightarrow \infty$, and U independent with huge degeneracies. The distribution of the eigenvalues is analogous to the spectrum of the $U/t \rightarrow \infty$ Hubbard model (t -model) on a complete graph [12,13] and, as shown later, this peculiar spectrum reflects the same underlying $\text{spl}(2,1)$ dynamical supersymmetry [12] (supersymmetry in the sense of odd and even number of fermions mixed in the same irreducible representation). For finite J_H/t the degeneracies are lifted except in the special case $U = J_H/2$ where some states with the same total spin value S remain degenerated as it can be realized in the qualitative comparison of Figs 1a and 1b. To understand this behavior: (a) we introduce Schwinger bosons to describe the spin degrees of freedom, and the form of the effective strong coupling Hamiltonian becomes remarkably simple, especially for $U = J_H/2$; (b) the effective strong coupling Hamiltonian is then solved exactly using dynamical supersymmetry and the $\text{spl}(2,1)$ graded algebra; (c) we show that in the limit $S_c \rightarrow \infty$ the semiclassical and quantum model give the same energy

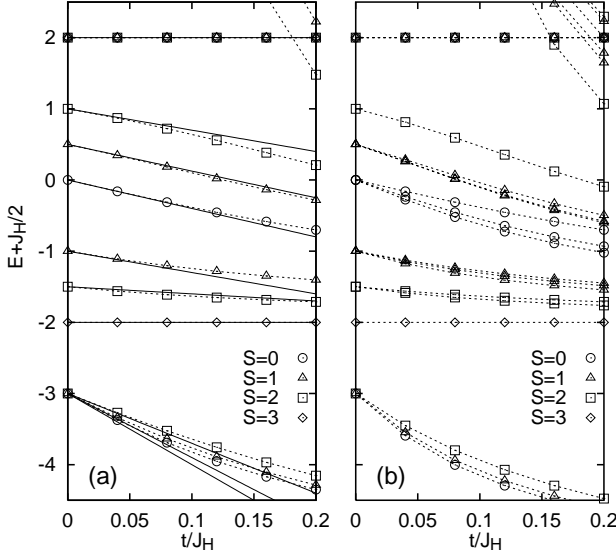


FIG. 1. The low energy spectrum of the ferromagnetic Kondo lattice on a 4 site complete graph with $S_c = 1/2$ and $N_e = 2$ for $U = J_H/2$ (a) and $U = 0$ (b). Each point is highly degenerate. The solid straight lines show the energy of the effective Hamiltonian as given by Eqs. (9)-(12).

spectrum, and that the semiclassical limit can be performed already at the level of the Kondo lattice Hamiltonian.

a. Effective strong coupling Hamiltonian. In the atomic limit ($t = 0$), the different lattice sites decouple. An empty site has energy 0; one electron can form with the core spin either the high ($S_c + 1/2$) or low ($S_c - 1/2$) spin state, with $E = -J_H S_c/2$ and $E = J_H(S_c + 1)/2$, respectively; finally two electrons results in a state with energy $E = U$ and spin S_c . This can be summarized by representing the different states using auxiliary fermions f and d and the spins by Schwinger bosons b_σ [14]:

$$\mathcal{H}_{\text{eff}} = -\frac{J_H N_e S_c}{2} - \frac{1}{2S_c + 1} \sum_{i,j,\alpha} t_{ij} f_i^\dagger b_{i\alpha}^\dagger b_{j\alpha} f_j - \frac{2}{J_H(2S_c + 1)^3} \sum_{i,j,k,\alpha,\beta} t_{ki} t_{ij} f_k^\dagger b_{k\alpha}^\dagger \left[\left(S_c + \frac{n_i^f}{2} \right) \delta_{\alpha\beta} - \mathbf{S}_i \cdot \boldsymbol{\sigma}_{\alpha\beta} \right] b_{j\beta} f_j \quad (3)$$

The first order term proportional to t in the expansion is equivalent to quantum double-exchange Hamiltonian derived by Kubo and Ohata [5] and by Müller-Hartmann and Dagotto [6]. Let us note here, that the procedure can be repeated for general U , and it would give us a more complicated t^2/J_H term [16].

b. The model on a complete graph. In this case, we can write the Hamiltonian (3) as

$$\mathcal{H}_{\text{eff}} = N_e \varepsilon_- - \frac{t}{2S_c + 1} \sum_{\alpha} F_{\alpha}^\dagger F_{\alpha} \quad (4)$$

$$- \frac{2t^2}{J_H(2S_c + 1)^3} \sum_{\alpha,\beta} F_{\alpha}^\dagger \left[\left(N S_c + \hat{N}_e/2 \right) \delta_{\alpha\beta} - \mathbf{S} \cdot \boldsymbol{\sigma}_{\alpha\beta} \right] F_{\beta},$$

$$c_{j\uparrow}^\dagger = \frac{1}{\sqrt{2S_c + 1}} \left(b_{j\uparrow}^\dagger f_j^\dagger + b_{j\downarrow}^\dagger d_j^\dagger \right),$$

$$c_{j\downarrow}^\dagger = \frac{1}{\sqrt{2S_c + 1}} \left(b_{j\downarrow}^\dagger f_j^\dagger - b_{j\uparrow}^\dagger d_j^\dagger \right).$$

where f^\dagger and d^\dagger are the creation operators of high and low spin states respectively while the spin operators in terms of Schwinger bosons are $S_j^z = (n_{j\uparrow}^b - n_{j\downarrow}^b)/2$, $S_j^+ = b_{j\uparrow}^\dagger b_{j\downarrow}$, and $S_j^- = b_{j\downarrow}^\dagger b_{j\uparrow}$. The anticommutation relation for electrons require the following constraint to be satisfied at each site

$$\sum_{\alpha} n_{j\alpha}^b - n_j^f + n_j^d = 2S_c.$$

In this representation the interaction part becomes diagonal

$$\mathcal{H}_{\text{int}} = \frac{J_H}{2} \sum_j \left[(S_c + 1) n_j^d - S_c n_j^f - n_j^f n_j^d \right] + U \sum_j n_j^f n_j^d.$$

Choosing $U = J_H/2$ we can eliminate the four fermion term $n_j^f n_j^d$. The effective strong coupling Hamiltonian is then the expansion in t/J_H around the atomic limit and is obtained using a canonical transformation. As a first step, following Ref. [15], we decompose the kinetic Hamiltonian into a part conserving the number of d and f fermions (\mathcal{T}_0), and a part where the final and initial state differs by a large energy $J_H(S_c + 1/2)$

$$\mathcal{T}_J = - \sum_{ij} \frac{t_{ij}}{2S_c + 1} \left(b_{i\downarrow} b_{j\uparrow} - b_{i\uparrow} b_{j\downarrow} \right) d_i^\dagger f_j,$$

so that $\mathcal{T} = \mathcal{T}_0 + \mathcal{T}_J + \mathcal{T}_J^\dagger$. The effective Hamiltonian is then given by $\mathcal{H}_{\text{eff}} = \mathcal{H}_{\text{int}} + \mathcal{T}_0 - [\mathcal{T}_J^\dagger, \mathcal{T}_J] / [(S_c + 1/2)J_H] + \mathcal{O}(t^3/J_H^2)$, and in the lowest energy subspace, where we keep the f fermions only, it reads

where $\varepsilon_- = t - J_H S_c/2$, and we introduced the fermionic operators $F_\alpha^\dagger = \sum_j b_{j\alpha}^\dagger f_j^\dagger$ and $F_\alpha = \sum_j b_{j\alpha} f_j$. with the nonvanishing anticommutation relations

$$\{F_\alpha^\dagger, F_\beta\} = \hat{Y} \delta_{\alpha\beta} + \mathbf{S} \cdot \boldsymbol{\sigma}_{\alpha\beta}, \quad (5)$$

where the spin operators $\mathbf{S} = \sum_j \mathbf{S}_j$ satisfy the usual

$$[S^+, S^-] = 2S^z, \quad [S^z, S^\pm] = \pm S^\pm, \quad (6)$$

su(2) spin algebra, and with the \hat{Y} operator defined as

$$\hat{Y} = (S_c + 1)N - \hat{N}_e/2, \quad [\mathbf{S}, \hat{Y}] = 0. \quad (7)$$

Finally, the commutation relations between the fermionic and bosonic operators read:

$$[F_\alpha, \mathbf{S}] = \frac{1}{2} \sum_\beta \boldsymbol{\sigma}_{\alpha\beta} F_\beta, \quad [F_\alpha, \hat{Y}] = -F_\alpha/2, \quad (8)$$

with their conjugate. The set of relations (5)-(8) define a $\text{spl}(2,1)$ graded algebra [17,18].

The rank of $\text{spl}(2,1)$ is 2, and we can define two linearly independent Casimir operators [17]:

$$\begin{aligned} \hat{C}_2 &= \mathbf{S}^2 - \hat{Y}^2 - \frac{1}{2} \sum_\alpha (F_\alpha^\dagger F_\alpha - F_\alpha F_\alpha^\dagger), \\ \hat{C}_3 &= \left(3\hat{C}_2 - \hat{S}^2 + \hat{Y}^2 - \hat{Y}\right) \left(\frac{\hat{Y}}{2} - \frac{1}{4}\right) + \frac{1}{2} \sum_{\alpha\beta} F_\alpha^\dagger \mathbf{S} \boldsymbol{\sigma}_{\alpha\beta} F_\beta. \end{aligned}$$

In general case the irreducible representation $[Y, S]$ is $8S$ dimensional and contains the (S, Y) , $(S-1/2, Y+1/2)$, $(S-1/2, Y-1/2)$ and $(S-1, Y)$ spin multiplets. Special cases concern the irreducible representation $[Y = S, S]$ which contains only the (S, Y) and $(S-1/2, Y+1/2)$ spin multiplets (dimension $4S+1$) and the irreducible

representation $[Y, S = 1/2]$ which do not contain the $(S-1, Y)$ spin multiplet. Applying operators F_α and F_α^\dagger we can walk between the different (S, Y) spin multiplets within an irreducible representation. The eigenvalues of the Casimir operators \hat{C}_2 and \hat{C}_3 are $S^2 - Y^2$ and $(S^2 - Y^2)Y$ in the irrep $[Y, S]$, respectively, while the eigenvalues of operators $\hat{\mathbf{S}}^2$ and \hat{Y} are $S'(S'+1)$ and Y' for an (S', Y') multiplet.

We can find the eigenvalues of the effective Hamiltonian using the representations of the $\text{spl}(2,1)$ superalgebra. The Hamiltonian conserves both the electron number and total spin: $[\mathcal{H}, \hat{Y}] = [\mathcal{H}, \mathbf{S}] = 0$, however it does not commute with the F 's. On the other hand, since $\sum_\alpha F_\alpha^\dagger F_\alpha = \hat{\mathbf{S}}^2 - \hat{Y}^2 + \hat{Y} - \hat{C}_2$, the $(S-1/2, Y-1/2)$, (S, Y) , $(S-1, Y)$, and $(S-1/2, Y+1/2)$ multiplets of the irreducible representation $[Y, S]$ are eigenstates of $\sum_\alpha F_\alpha^\dagger F_\alpha$ with the eigenvalues $2Y-1$, $Y+S$, $Y-S$, and 0, respectively. Similarly, the \hat{C}_3 appears in the t^2/J_H corrections in the Hamiltonian. Finally, the effective Hamiltonian turns out to be a combination of \hat{C}_2 , \hat{C}_3 , $\hat{\mathbf{S}}^2$ and \hat{Y} , and the states $|(S, Y)_{[Y', S']}\rangle$ are eigenstates with (increasing) energies:

$$E_{[Y+1/2, S+1/2]}(S, Y) = N_e \varepsilon_- - 2 \left(t + \frac{2t^2}{J_H} \frac{S^{\max} + 1}{(2S_c + 1)^2} \right) \left(N - \frac{S^{\max}}{2S_c + 1} \right) + \frac{4t^2}{J_H} \frac{S(S+1)}{(2S_c + 1)^3} + \mathcal{O}\left(\frac{t^3}{J_H^2}\right), \quad (9)$$

$$E_{[Y, S]}(S, Y) = N_e \varepsilon_- - \left(t + \frac{2t^2}{J_H} \frac{S^{\max} - S}{(2S_c + 1)^2} \right) \left(N - \frac{S^{\max} - S}{2S_c + 1} \right) + \mathcal{O}\left(\frac{t^3}{J_H^2}\right), \quad (10)$$

$$E_{[Y, S+1]}(S, Y) = N_e \varepsilon_- - \left(t + \frac{2t^2}{J_H} \frac{S^{\max} + S + 1}{(2S_c + 1)^2} \right) \left(N - \frac{S^{\max} + S + 1}{2S_c + 1} \right) + \mathcal{O}\left(\frac{t^3}{J_H^2}\right), \quad (11)$$

$$E_{[Y-1/2, S+1/2]}(S, Y) = N_e \varepsilon_-, \quad (12)$$

where $S^{\max} = NS_c + N_e/2 = (2S_c + 1)N - Y$ is the maximum total spin. In Fig. 1 these energies are compared with those of the Kondo lattice for $U = J_H/2$ at left. It appear that the computed correction is the correct one but for $t/J_H > 0.05$ higher terms are necessary. It is interesting to note that the $E_{[Y-1/2, S+1/2]}(S, Y) = \varepsilon_- - N_e$ is the eigenvalue for any J_H . To obtain this solution it is essential that the effective Hamiltonian can be expressed using the operators of the $\text{spl}(2,1)$ superalgebra which, for finite J_H/t , is possible for $U = J_H/2$ only.

Let us now address the question of the degeneracy of each level. For one site, the states with $S = S_c$ and $S_c + 1/2$ form the irreducible representation $[S_c + 1/2, S_c + 1/2]$. With N sites, the degeneracy $M_{[Y, S]}^{(N)}$ is determined by the number of times the irrep $[Y, S]$ is contained in $[S_c + 1/2, S_c + 1/2]^N$. This is determined from the branching rule [17], leading to the following recursion relation:

$$M_{[Y, S+1/2]}^{(N+1)} = \sum_{y=\{0, 1/2\}} \sum_{s=-S_c-y}^{S-|S-y-S_c|} M_{[Y+y-S_c-1, S-s+1/2]}^{(N)},$$

with $M_{[Y=N(S_c+1/2), S]}^{(N)} = \delta_{S, N(S_c+1/2)}$ as boundary condition. This recursion formula along with the energy def-

inition in Eqs. (9)-(12) allows an iterative procedure to build the energy density distribution of the model. In Tab. I we show as an example the spectrum of the 4 site cluster.

For $N_e = 1$ the (S, Y) spin multiplet of the $[Y+1/2, S+1/2]$ is missing and the ground state is the highest spin state in the $[Y, S]$ irrep. For $1 < N_e \leq N$ the t/J_H correction makes the lowest energy state to be the singlet in the $[Y+1/2, 1/2]$ irrep, and the low energy spectrum behaves as $S(S+1)$, like in the antiferromagnetic infinite range Heisenberg model. For $N_e > N$ we can use that $E(N_e, t, J_H) = E(2N - N_e, -t, J_H) + U(N_e - N)$, and from this we obtain that when $N_e = N + 1$ the ground state is again the highest spin state (a similar situation is encountered in the Hubbard model [19]). Finally, for $N + 1 < N_e < 2N$ the ground state is highly degenerate and the corresponding energy can be obtained from Eq. (12) with the appropriate change. To summarize, the highest spin multiplet is the non degenerate ground state for $N_e = 1$ and $N_e = N + 1$ only, cases referred to true ferromagnetism.

c. Semiclassical limit. In the limit $S_c \rightarrow \infty$ we can replace \mathbf{S}_j by $S_c(\sin \theta_j \cos \phi_j, \sin \theta_j \sin \phi_j, \cos \theta_j)$ in the

Kondo Hamiltonian (2) with $J = J_H(S_c + 1/2)$ fixed, and we end up with an noninteracting model [20]. The one-particle spectrum comes out as follows: two $N - 2$ degenerate states with energy $\varepsilon_{\pm} = t \pm J/2$ and four nondegenerate states with energies

$$\varepsilon_{s_1 s_2} = -\frac{N-2}{2}t + \frac{s_1}{2}\sqrt{J^2 + N^2 t^2 - 2s_2 J t \frac{S}{S_c}},$$

where s_1 and s_2 are ± 1 . The lowest energy state corresponds to $s_1 = -1$ and $s_2 = -1$, and for $J_H \gg t$ the energy is linearly decreasing with S , i.e. the fermions can freely propagate when the spins are parallel. In the next state (ε_{-+}) the tendency is reversed: energy is higher for larger S . The absence of the true ferromagnetic state can be traced to the cancelation of the contributions linear in S for $N_e > 2$. This does not happen in a model with less pathological one-particle spectrum, e.g on the cubic lattice the ferromagnetism is realized for a wide range of hole concentration [8]. Filling the one-particle levels, the lowest part of the spectrum for $1 < N_e \leq N$ electron is $\varepsilon_{--} + \varepsilon_{-+} + (N_e - 2)\varepsilon_{-}$, $\varepsilon_{--} + (N_e - 1)\varepsilon_{-}$, $\varepsilon_{-+} + (N_e - 1)\varepsilon_{-}$, and $N_e \varepsilon_{-}$. These energies are equal, up to corrections $\mathcal{O}(t^3/J^2, 1/S_c)$, to the energies (9)-(12) of the (S, Y) spin multiplet in the $[Y + 1/2, S + 1/2]$, $[Y, S]$, $[Y, S + 1]$, and $[Y - 1/2, S + 1/2]$ irreps, respectively. This way we can establish a one-to-one correspondence between the semiclassical and quantum spectra for this particular model.

To conclude, we have shown that the effective strong coupling limit of the Kondo lattice model on a complete graph can be described by the $\text{spl}(2,1)$ graded algebra and exhibits a dynamical supersymmetry. In contrast to Hubbard model, the supersymmetry is not limited to the t -model only, but holds also in the next order (t^2/J_H) for a special value of on-site repulsion. This, and the numerical diagonalization on small clusters suggest that not only the strong coupling limit, but the Kondo Hamiltonian itself is supersymmetric. We also show that for $S_c \rightarrow \infty$ the spectrum of quantum model can be derived from one-particle states of the semiclassical Kondo lattice model. Finally, the ferromagnetic ground state is reduced to the case when we have only 1 or $N+1$ electron, in contrary to the generally accepted expectations.

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$N_e(Y)$	0(6)	1(11/2)	2(5)	3(9/2)	4(4)
E' 2S	4 2 0	5 3 1	6 4 2 0	7 5 3 1	8 6 4 2 0
0	1 3 2	3 <u>8</u> 7	3 6 6 3	1	
-1/2				3	
-1			3	6	
-3/2		1	<u>8</u>	6	
-2		3	7		
-5/2				3	
-3		2	7	6	
-7/2		3	<u>8</u>	6	
-4		1	3	3	1 3 6 6 3
-9/2				3 <u>8</u> 7	
-5			1 3 2		

TABLE I. The spectrum and multiplicities of the quantum double exchange ($J_H/t \rightarrow +\infty$) for $S_c = 1/2$ and $N = 4$. Here $E' = E - N_e \varepsilon_{-}$. As an example, we have underlined the four spin multiplets of the $[Y = 5, S = 2]$ irreducible representation, which has multiplicity 8.